

# High Resolution Data Collection for Crystals of a Recombinant Antigen-Binding Fragment Complexed with Single-stranded DNA

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Abstract No. Tann0386

Beamline(s): X8C, X12B

**Introduction:** Anti-DNA antibodies have been implicated in autoimmune diseases such as systemic lupus erythematosus. High-resolution crystal structures of anti-DNA antibodies are important because they serve as templates for designing inhibitor molecules that could be potentially useful in treating lupus. Crystals of a recombinant antigen-binding fragment (Fab) complexed with dT<sub>5</sub> have been obtained and the structure has been determined using data collected at two NSLS beamlines.

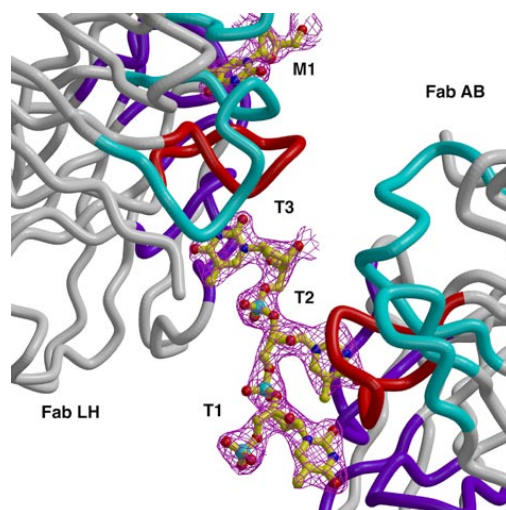
**Results:** The crystals occupy space group P6<sub>5</sub>22 with a=171.8 Å, c=144.6 Å, and there are two Fab per asymmetric unit. These crystals diffract to only 2.5 Å resolution using a rotating anode X-ray source, therefore, the high-resolution data that was needed could only be obtained at a synchrotron facility.

X-ray diffraction data were collected to 2.1 Å resolution from two crystals at beamlines X8C and X12B of the National Synchrotron Light Source at Brookhaven National Laboratory. A total of 68° of data were collected at the two beamlines using Quantum 4 CCD detectors with an oscillation angle of 0.25-0.5°, an exposure time of 10 minutes per degree of oscillation, a detector distance of either 200 mm or 220 mm and a detector offset angle of zero. The merged data set is 99% complete to 2.1 Å resolution, with an R<sub>sym</sub> on I of 0.079,  $\langle I/\sigma(I) \rangle$  of 19.3, and average multiplicity of 6.8. Phases have been determined using molecular replacement and the structure has been refined to R-work = 0.225 and R-free = 0.260.

**Acknowledgments:** This work was supported in part by a grant from the University of Missouri Research Board.

**References:** S.P. Prewitt, A.A. Komissarov, S.L. Deutscher, and J.J. Tanner, "Crystallization and Molecular Replacement Studies of a Recombinant Antigen-Binding Fragment Complexed with Single-stranded DNA,"

Acta Cryst. **D56**, 1007-1011, 2000.



**Figure 1.** Close-up view of the two Fab molecules in the asymmetric unit. Note that both Fabs contact the same fragment of DNA.